APPENDIX A-1b

CHEMICAL AND PHYSICAL PROPERTIES AND TOXICITY REFERENCE LEVELS

TABLE A-1b-1

CHEMICAL-SPECIFIC INPUTS FOR ACENAPTHYLENE (208-96-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	152.20
T_m (K)	CRC Handbook (1995)	365.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was cited from CRC Handbook (1995).	8.29E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.39E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.53E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.55E-01
t	*t* value was obtained from U.S. EPA (1992b).	7.42E-01
*t**	t* value was obtained from U.S. EPA (1992b).	6.23E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.00E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-1

CHEMICAL-SPECIFIC INPUTS FOR ACENAPTHYLENE (208-96-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	6.00E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	2.1E-01
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-2

CHEMICAL-SPECIFIC INPUTS FOR ACRYLAMIDE (79-06-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	71.08
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	357.65
Vp (atm)	*Vp* value cited in U.S. EPA (1995g)	9.20E-06
S (g/100ml H_2O)	Geometric mean value cited in U.S. EPA (1994c).	2.15E+02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g)	3.00E-10
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.70E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.06E-05
K_{ow} (unitless)	--	1.10E-01
K_{oc} (mL/g)	--	1.10E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.10E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.00E-03
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.50E-04
t	*t* value was obtained from U.S. EPA (1992b).	2.40E-01
*t**	t* value was obtained from U.S. EPA (1992b).	5.70E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.10E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	7.70E-02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-2

CHEMICAL-SPECIFIC INPUTS FOR ACRYLAMIDE (79-06-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1997b)	2.00E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S.EPA (1997b)	4.50E+00
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.00E-04
Inhalation CSF $(mg/kg/day)^{-1}$	U.S.EPA (1997b)	4.55E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-3

CHEMICAL-SPECIFIC INPUTS FOR ALLYL CHLORIDE (107-05-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	76.53
T_m (K)	Montgomery and Welkom (1991)	138.65
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	4.80E-01
S (mg/L)	*S* value cited in U.S. EPA (1995g).	3.40E+03
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g)	1.10E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.17E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.08E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	2.80E+01
K_{oc} (mL/g)	K_{cw} value cited in U.S. EPA (1995g).	2.70E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.70E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.02E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	7.00E-03
t	*t* value was obtained from U.S. EPA (1992b).	2.60E-01
*t**	t* value was obtained from U.S. EPA (1992b).	6.20E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.80E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.70E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-3

CHEMICAL-SPECIFIC INPUTS FOR ALLYL CHLORIDE (107-05-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	2.86E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	1.0E-03
Inhalation [1] *CSF* $(mg/kg/day)^{-}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-4

CHEMICAL-SPECIFIC INPUTS FOR BENZIDINE (92-87-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	184.23
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	390.65
Vp (atm)	--	ND
S (g/2500ml)	Geometric mean value cited in U.S. EPA (1994c).	1.0
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.88E-11
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.50E-05
K_{ow} (unitless)	--	4.60E+01
K_{oc} (mL/g)	--	4.30E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.30E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.22E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.20E-03
t	*t* value was obtained from U.S. EPA (1992b).	1.20E+00
*t**	t* value was obtained from U.S. EPA (1992b).	2.80E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.60E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.00E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-4

CHEMICAL-SPECIFIC INPUTS FOR BENZIDINE (92-87-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1997b)	3.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	2.30E+02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.10E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	2.35E+02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1995f)	2.5E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1b-5

CHEMICAL-SPECIFIC INPUTS FOR BENZO(GHI)PERYLENE (191-24-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	276.34
T_m (°K)	--	ND
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	7.40229E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	2.01E-02
D_w (cm^2/s)	D_W value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	5.26E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (mL/g)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.62E+00
t	*t* value was obtained from U.S. EPA (1992b).	4.24E+00
*t**	t* value was obtained from U.S. EPA (1992b).	2.00E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.16E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-5

CHEMICAL-SPECIFIC INPUTS FOR BENZO(GHI)PERYLENE (191-24-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-6

CHEMICAL-SPECIFIC INPUTS FOR BIS-(2-CHLOROETHOXY) METHANE (111-91-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1990)	173.04
T_m (°K)	Montgomery and Welkom (1990)	240.35
Vp (1mm @53 °C)	Montgomery and Welkom (1990)	1.0
S (mg/L@ 25 °C)	All metals, except mercury, are assumed to be insoluble in water.	81,000.00
H (atm·m^3/mol)	U.S. EPA (1998c)	3.78E-07
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	3.20E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.46E-06
K_{ow} (unitless)	Montgomery and Welkom (1990)	1.82E+01
K_{oc} (mL/g)	Montgomery and Welkom (1990)	1.14E+02
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.14E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.55E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	131E-03
t	*t* value was obtained from U.S. EPA (1992b).	9.95E-01
*t**	t* value was obtained from U.S. EPA (1992b).	2.39E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.82E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-6

CHEMICAL-SPECIFIC INPUTS FOR BIS-(2-CHLOROETHOXY) METHANE (111-91-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-7

CHEMICAL-SPECIFIC INPUTS FOR BUTANOL (71-36-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1995g)	74.12
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	8.60E-03
S (mg/L)	U.S. EPA (1995g)	7.50E+04
H (atm·m^3/mol)	U.S. EPA (1995g)	8.81E-06
D_a (cm^2/s)	U.S. EPA (1995g)	8.00E-02
D_w (cm^2/s)	U.S. EPA (1995g)	9.30E-06
K_{ow} (unitless)	U.S. EPA (1995g)	6.30E+00
K_{oc} (mL/g)	U.S. EPA (1995g)	6.10E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.10E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.58E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.50E-03
t	*t* value was obtained from U.S. EPA (1992b).	2.50E-01
*t**	t* value was obtained from U.S. EPA (1992b).	5.90E-01
B	*B* value was obtained from U.S. EPA (1992b).	6.30E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.20E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-7

CHEMICAL-SPECIFIC INPUTS FOR BUTANOL (71-36-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	1.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.50E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-8

CHEMICAL-SPECIFIC INPUTS FOR BUTYL-4,6-DINITROPHENOL, 2-SEC (DINOSEB) (88-85-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	240.22
T_m (K)	U.S. EPA (1995b)	311.15 to 414.15
Vp (atm)	U.S. EPA (1995g)	9.90E-05
S (mg/L)	U.S. EPA (1995g)	5.20E+01
H (atm·m^3/mol)	U.S. EPA (1995g)	4.56E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
K_{ow} (unitless)	U.S. EPA (1995g)	1.40E+03
K_{oc} (mL/g)	U.S. EPA (1995g)	1.20E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.20E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.00E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
t	*t* value was obtained from U.S. EPA (1992b).	2.60E+00
*t**	t* value was obtained from U.S. EPA (1992b).	8.30E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.40E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	8.00E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-8

CHEMICAL-SPECIFIC INPUTS FOR BUTYL-4,6-DINITROPHENOL, 2-SEC (DINOSEB) (88-85-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	1.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.50E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-9

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORO-1,3-BUTADIENE (CHLOROPRENE) (126-99-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1995g)	88.54
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	2.80E-01
S (mg/L)	U.S. EPA (1995g)	6.30E+02
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.04E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.00E-05
K_{ow} (unitless)	U.S. EPA (1995g)	1.20E+02
K_{oc} (mL/g)	U.S. EPA (1995g)	1.10E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table. 5g)	1.10E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.25E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.60E-02
t	*t* value was obtained from U.S. EPA (1992b).	3.00E-01
*t**	t* value was obtained from U.S. EPA (1992b).	7.30E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.20E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.10E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-9

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORO-1,3-BUTADIENE (CHLOROPRENE) (126-99-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	2.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (1997b)	2.00E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-10

CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (+3) (16065-38-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	51.996
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	2173.15
Vp (atm)	--	0
S (mg/L)	--	0
H (atm·m^3/mol)	--	0
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.01E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	4.63E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e).	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
t	*t* value was obtained from U.S. EPA (1992b).	ND
*t**	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-10

CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (+3) (16065-38-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note:NA = Not applicable, ND = No data available

TABLE A-1b-11

CHEMICAL-SPECIFIC INPUTS FOR CIS-1,3-DICHLOROPROPENE (10061-01-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	110.97
T_m (^{o}K)	--	
Vp (atm)	U.S. EPA (1995g)	4.99E-02
S (mg/L)	U.S. EPA (1995g)	2.70E+03
H (atm·m^3/mol)	U.S. EPA (1995g)	1.76E-03
D_a (cm^2/s)	U.S. EPA (1995g)	5.85E-02
D_w (cm^2/s)	U.S. EPA (1995g)	1.10E-05
K_{ow} (unitless)	U.S. EPA (1995g)	1.00E+02
K_{oc} (mL/g)	U.S. EPA (1995g)	9.30E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.30E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.97E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
t	*t* value was obtained from U.S. EPA (1992b).	4.20E-01
*t**	t* value was obtained from U.S. EPA (1992b).	1.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.00E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	5.30E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-11

CHEMICAL-SPECIFIC INPUTS FOR CIS-1,3-DICHLOROPROPENE (10061-01-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	1.75E-01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	1.75E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1995f)	2.40E+01

Note: Not applicable, ND = No data available

TABLE A-1b-12

CHEMICAL-SPECIFIC INPUTS FOR COBALT (7440-48-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	58.93
T_m (K)	Montgomery and Welkom (1991)	1766.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
t	*t* value was obtained from U.S. EPA (1992b).	ND
*t**	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-12

CHEMICAL-SPECIFIC INPUTS FOR COBALT (7440-48-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1997b)	6.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	2.10E-01
Inhalation CSF $(mg/kg/day)^{-1}$	.	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-13

CHEMICAL-SPECIFIC INPUTS FOR COPPER (744-050-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	63.55
T_m (K)	Montgomery and Welkom (1991)	1356.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	2.20E+01
Kd_{sw} (L/Kg)	--	2.20E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
t	*t* value was obtained from U.S. EPA (1992b).	ND
*t**	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	0.0E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-13

CHEMICAL-SPECIFIC INPUTS FOR COPPER (744-050-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1997b)	4.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.40E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	1.3
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	9.00E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1b-14

CHEMICAL-SPECIFIC INPUTS FOR CYCLOTETRAMETHYLENETETRANITRAMINE (HMX) (2691-41-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	296.16
T_m (K)	CRC Handbook (1995)	559.15
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from WATER8 model database (U.S. EPA 1995d).	2.60E-15
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	8.00E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.28E-05
t	*t* value was obtained from U.S. EPA (1992b).	6.90E-01
*t**	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-14

CHEMICAL-SPECIFIC INPUTS FOR CYCLOTETRAMETHYLENETETRANITRAMINE (HMX) (2691-41-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	5.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.75E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-15

CHEMICAL-SPECIFIC INPUTS FOR DIALLATE (2303-16-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	270.24
T_m (K)	--	ND
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	2.00E-07
S (ppm)	*S* value cited in U.S. EPA (1995b).	40
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.83E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
K_{ow} (unitless)	Value cited in U.S. EPA (1995g).	3.10E+04
K_{oc} (mL/g)	Value cited in U.S. EPA (1995g).	2.60E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.60E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.82E+03
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	6.60E-02
t	*t* value was obtained from U.S. EPA (1992b).	3.90E+00
*t**	t* value was obtained from U.S. EPA (1992b).	2.00E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.10E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	1.80E+04

TABLE A-1b-15

CHEMICAL-SPECIFIC INPUTS FOR DIALLATE (2303-16-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	6.10E-02
RfC (mg/m^3)	--	ND
Inhalation URF $(\mu g/m^3)^{-1}$	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	6.10E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA= Not applicable, ND= No data available

TABLE A-1b-16

CHEMICAL-SPECIFIC INPUTS FOR DIBENZOFURAN (132-64-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	168.19
T_m (K)	CRC Handbook (1995)	359.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.056E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.06E-01
t	*t* value was obtained from U.S. EPA (1992b).	6.90E-01
*t**	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	2.04E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-16

CHEMICAL-SPECIFIC INPUTS FOR DIBENZOFURAN (132-64-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1997a)	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1996c)	2.00E+1

Note: NA = Not applicable, ND = No data available

TABLE A-1b-17

CHEMICAL-SPECIFIC INPUTS FOR 2,6-DICHLOROPHENOL (87-65-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	163.01
T_m (K)	Howard (1989-1993)	337.65 to 338.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.96E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.47E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.77E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.07E-02
t	*t* value was obtained from U.S. EPA (1992b).	8.63E-01
*t**	t* value was obtained from U.S. EPA (1992b).	2.07E+00
B	*B* value was obtained from U.S. EPA (1992b).	7.24E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-17

CHEMICAL-SPECIFIC INPUTS FOR 2,6-DICHLOROPHENOL (87-65-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-18

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOXYACETIC ACID (94-75-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1995g)	221.04
T_m (K)	--	ND
Vp (atm)	U.S. EPA (1995g)	1.40E-05
S (mg/L)	U.S. EPA (1995g)	6.80E+02
H (atm·m^3/mol)	U.S. EPA (1995g)	4.50E-06
D_a (cm^2/s)	U.S. EPA (1995g)	5.88E-02
D_w (cm^2/s)	U.S. EPA (1995g)	6.49E-06
K_{ow} (unitless)	U.S. EPA (1995g)	5.05E+02
K_{oc} (mL/g)	U.S. EPA (1995g)	4.50E+02
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.--	4.50E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.37E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	7.10E-03
t	*t* value was obtained from U.S. EPA (1992b).	2.00E+00
*t**	t* value was obtained from U.S. EPA (1992b).	4.70E+00
B	*B* value was obtained from U.S. EPA (1992b).	5.00E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	6.10E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-18

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOXYACETIC ACID (94-75-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	1.00E-02
Oral CSF $(mg/kg/day)^{-1}$	Calculated by multiplying the Oral CSF for Benzo(a)pyrene by the relative potency factor for Dibenz(a,h)anthracene of 1.0 (U.S.EPA 1993e).	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.50E-02
Inhalation CSF $(mg/kg/day)^{-1}$		ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-19

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROPROPENE-TRANS (10061-02-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	110.98
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	4.00E-02
S (mg/L)	U.S. EPA (1995g)	2.80E+03
H (atm·m^3/mol)	U.S. EPA (1995g)	1.25E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.85E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
K_{ow} (unitless)	U.S. EPA (1995g)	1.00E+02
K_{oc} (mL/g)	U.S. EPA (1995g)	9.30E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.30E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.97E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
t	*t* value was obtained from U.S. EPA (1992b).	4.20E-01
*t**	t* value was obtained from U.S. EPA (1992b).	1.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.00E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	5.30E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-19

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROPROPENE-TRANS (10061-02-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	1.75E-01
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	1.75E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1995f)	2.40E+01

Note: NA= Not applicable, ND= No data available

TABLE A-1b-20

CHEMICAL-SPECIFIC INPUTS FOR DIETHYLSTILBESTROL (56-53-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	268.34
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	443.65
Vp (atm)	U.S. EPA (1995g)	1.40E-12
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.30E+04
H (atm·m^3/mol)	U.S. EPA (1995g)	3.00E-14
D_a (cm^2/s)	U.S. EPA (1995g)	8.00E-02
D_w (cm^2/s)	U.S. EPA (1995g)	8.00E-06
K_{ow} (unitless)	U.S. EPA (1995g)	1.20E+05
K_{oc} (mL/g)	U.S. EPA (1995g)	9.60E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.60E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.20E+03
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.70E-01
t	*t* value was obtained from U.S. EPA (1992b).	3.80E+00
*t**	t* value was obtained from U.S. EPA (1992b).	1.80E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.20E+01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	6.80E+03

TABLE A-1b-20

CHEMICAL-SPECIFIC INPUTS FOR DIETHYLSTILBESTROL (56-53-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1996d)	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	4.70E+03
RfC (mg/m^3)	U.S. EPA (1997b)	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-21

CHEMICAL-SPECIFIC INPUTS FOR DIMETHOATE (60-51-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	229.28
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	6.70E-09
S (mg/L)	U.S. EPA (1995g)	2.50E+04
H (atm·m^3/mol)	U.S. EPA (1995g)	6.15E-11
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.58E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.82E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	4.90E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.80E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.80E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.60E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.40E-04
t	*t* value was obtained from U.S. EPA (1992b).	2.20E+00
*t**	t* value was obtained from U.S. EPA (1992b).	5.30E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.90E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	8.40E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-21

CHEMICAL-SPECIFIC INPUTS FOR DIMETHOATE (60-51-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1997c)	2.00E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.00E-04
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA= Not applicable, ND= No data available

TABLE A-1b-22

CHEMICAL-SPECIFIC INPUTS FOR 7,12-DIMETHYLBENZ[A]ANTHRACENE (57-97-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	256.35
T_m (K)	--	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.80E-12
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.00E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.11E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.61E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.98E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	4.20E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.20E+06
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.20E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.40E+05
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.60E+00
t	*t* value was obtained from U.S. EPA (1992b).	3.20E+00
*t**	t* value was obtained from U.S. EPA (1992b).	1.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	4.20E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)-	1.00E+03

TABLE A-1b-22

CHEMICAL-SPECIFIC INPUTS FOR 7,12-DIMETHYLBENZ[A]ANTHRACENE (57-97-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	2.50E+01
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	2.50E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA= Not applicable, ND= No data available

TABLE A-1b-23

CHEMICAL-SPECIFIC INPUTS FOR 3-3'-DIMETHYLBENZIDINE (119-93-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	212.28
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.90E-10
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.20E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.29E-11
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.83E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.17E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	4.80E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.30E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.30E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.22E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	7.70E-03
t	*t* value was obtained from U.S. EPA (1992b).	1.70E+00
*t**	t* value was obtained from U.S. EPA (1992b).	4.10E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.80E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.80E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-23

CHEMICAL-SPECIFIC INPUTS FOR 3-3'-DIMETHYLBENZIDINE (119-93-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	9.20E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	9.20E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA= Not applicable, ND= No data available

TABLE A-1b-24

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITRO-6-METHYLPHENOL (534-52-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	198.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	360.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.26E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.93E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.91E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.78E-03
t	*t* value was obtained from U.S. EPA (1992b).	1.41E+00
*t**	t* value was obtained from U.S. EPA (1992b).	3.39E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.32E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-24

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITRO-6-METHYLPHENOL (534-52-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-25

CHEMICAL-SPECIFIC INPUTS FOR DIPHENYLAMINE (122-39-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	169.23
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.60E-06
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.00E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.96E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.31E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	3.00E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.60E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.60E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.95E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	5.20E-02
t	*t* value was obtained from U.S. EPA (1992b).	9.40E-01
*t**	t* value was obtained from U.S. EPA (1992b).	5.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.00E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	8.30E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-25

CHEMICAL-SPECIFIC INPUTS FOR DIPHENYLAMINE (122-39-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	2.50E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	8.82E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-26

CHEMICAL-SPECIFIC INPUTS FOR 2-ETHOXYETHANOL (110-80-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	90.12
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.00E-03
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.20E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.23E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.47E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.57E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	7.90E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.00E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.00E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.00E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.60E-04
t	*t* value was obtained from U.S. EPA (1992b).	3.10E-01
*t**	t* value was obtained from U.S. EPA (1992b).	7.40E-01
B	*B* value was obtained from U.S. EPA (1992b).	7.90E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.20E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-26

CHEMICAL-SPECIFIC INPUTS FOR 2-ETHOXYETHANOL (110-80-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	Calculated from *RfC* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	5.70E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (1997c)	2.00E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-27

CHEMICAL-SPECIFIC INPUTS FOR ETHYL ACETATE (141-78-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	88.1
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.20E-01
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.40E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.38E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.32E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.66E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	4.90E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.80E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.80E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.60E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.70E-03
t	*t* value was obtained from U.S. EPA (1992b).	3.00E-01
*t**	t* value was obtained from U.S. EPA (1992b).	7.20E-01
B	*B* value was obtained from U.S. EPA (1992b).	4.90E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	9.90E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-27

CHEMICAL-SPECIFIC INPUTS FOR ETHYL ACETATE (141-78-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	9.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg. 1997c)	3.15E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-28

CHEMICAL-SPECIFIC INPUTS FOR ETHYL ETHER (60-29-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	74.12
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.10E-01
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.10E+04
H (atm·m^3/mol)	U.S. EPA (1995g)	8.70E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.40E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	6.80E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.50E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.50E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.88E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.60E-03
t	*t* value was obtained from U.S. EPA (1992b).	2.50E-01
*t**	t* value was obtained from U.S. EPA (1992b).	5.90E-01
B	*B* value was obtained from U.S. EPA (1992b).	6.80E-04
Biotransfer Factors for Animals		
BCF_{fish} (L//kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.30E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-28

CHEMICAL-SPECIFIC INPUTS FOR ETHYL ETHER (60-29-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1996b)	2.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.00E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA= Not applicable, ND= No data available

TABLE A-1b-29

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE THIOUREA (ETU) (96-45-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	102.17
T_m (°K)	Budavari, O'Neill, Smith, and Heckelman (1989)	476.65
Vp	Geometric mean value cited in U.S. EPA (1994c).	1.10E-04
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.20E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.08E-10
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.15E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.02E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.20E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.20E-01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.20E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.65E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.50E-04
t	*t* value was obtained from U.S. EPA (1992b).	3.70E-01
*t**	t* value was obtained from U.S. EPA (1992b).	8.80E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.20E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	7.90E-02
BAF_{fish} (L/kg FW)	--	NA

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	Value based on Inhalation CSF assuming route-to-route extrapolation.	1.10E-01
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	1.10E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: ND= Not applicable, ND= No data available

TABLE A-1b-30

CHEMICAL-SPECIFIC INPUTS FOR FURAN (110-00-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	68.08
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.90E-01
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.00E+04
H (atm·m^3/mol)	U.S. EPA (1995g)	5.40E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.04E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.22E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.20E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.10E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.10E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.57E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	6.50E-03
t	*t* value was obtained from U.S. EPA (1992b).	2.30E-01
*t**	t* value was obtained from U.S. EPA (1992b).	5.50E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.20E-03
Biotransfer Factors for Animals		
BCF_{fish} (unitless, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.00E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-30

CHEMICAL-SPECIFIC INPUTS FOR FURAN (110-00-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	1.00-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.50E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-31

CHEMICAL-SPECIFIC INPUTS FOR GAMMA-HEXACHLOROCYCLOHEXANE (LINDANE) (58-89-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.85
T_m (K)	Montgomery and Welkom (1991)	385.65
Vp (mmHG)	Geometric mean value cited in U.S. EPA (1994c).	9.40 E-06
S (in water)	U.S. EPA (1995g)	4.20E+00
H (atm·m^3/mol)	U.S. EPA (1995g).	3.40E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.42E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.34E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	5.40E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.60E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.60E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.45E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.40E-02
t	*t* value was obtained from U.S. EPA (1992b).	5.20E+00
*t**	t* value was obtained from U.S. EPA (1992b).	3.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.40E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	1.60E+03

TABLE A-1b-31

CHEMICAL-SPECIFIC INPUTS FOR GAMMA-HEXACHLOROCYCLOHEXANE (LINDANE) (58-89-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1997b)	3.00E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S.EPA (1997b)	1.30E+00
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.05E-03
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	1.30E+00
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (µg/l)	U.S. EPA (1995f)	8E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1b-32

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPROPENE (1888-71-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	248.75
T_m (K)	CRC Handbook (1995)	200.25
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from WATER8 model database (U.S. EPA 1995d).	4.70E-03
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	8.00E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
t	*t* value was obtained from U.S. EPA (1992b).	2.88E+00
*t**	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-32

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPROPENE (1888-71-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA= Not applicable, ND= No data available

TABLE A-1b-33

CHEMICAL-SPECIFIC INPUTS FOR IRON (7439-89-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	55.84
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	1808.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
t	*t* value was obtained from U.S. EPA (1992b).	1.00E-03
*t**	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-33

CHEMICAL-SPECIFIC INPUTS FOR IRON (7439-89-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1997b)	3.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.05E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--.	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.0E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1b-34

CHEMICAL-SPECIFIC INPUTS FOR ISOBUTYL ALCOHOL (78-83-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	74.14
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.40E-02
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.60E+04
H (atm·m^3/mol)	U.S. EPA (1995g)	1.30E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.60E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.60E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.50E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.50E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.13E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.30E-03
t	*t* value was obtained from U.S. EPA (1992b).	2.50E-01
*t**	t* value was obtained from U.S. EPA (1992b).	5.90E-01
B	*B* value was obtained from U.S. EPA (1992b).	5.60E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.00E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-34

CHEMICAL-SPECIFIC INPUTS FOR ISOBUTYL ALCOHOL (78-83-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	3.00E-01
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.05E+00
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-35

CHEMICAL-SPECIFIC INPUTS FOR KEPONE (143-50-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	490.68
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.90E-10
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.60E+00
H (atm·m^3/mol)	U.S. EPA (1995g)	2.55E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.00E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.60E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.60E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.20E+04
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
t	*t* value was obtained from U.S. EPA (1992b).	8.60E+01
*t**	t* value was obtained from U.S. EPA (1992b).	4.10E+02
B	*B* value was obtained from U.S. EPA (1992b).	2.00E+01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	1.80E+03

TABLE A-1b-35

CHEMICAL-SPECIFIC INPUTS FOR KEPONE (143-50-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	1.80E+01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	1.80E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-36

CHEMICAL-SPECIFIC INPUTS FOR MAGNESIUM (7439-95-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	24.30
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	924.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
t	--	ND
*t**	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-36

CHEMICAL-SPECIFIC INPUTS FOR MAGNESIUM (7439-95-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-37

CHEMICAL-SPECIFIC INPUTS FOR MANGANESE (7439-96-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	54.94
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1517.15
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	8.00E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
t	--	ND
*t**	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-37

CHEMICAL-SPECIFIC INPUTS FOR MANGANESE (7439-96-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1996c)	8.00E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1b-38

CHEMICAL-SPECIFIC INPUTS FOR 3-METHYLCHOLANTHRENE (56-49-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	268.34
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	452.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.4E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.09E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.36E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.60E+00
t	*t* value was obtained from U.S. EPA (1992b).	3.80E+00
*t**	t* value was obtained from U.S. EPA (1992b).	1.80E+01
B	*B* value was obtained from U.S. EPA (1992b).	2.60E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	1.96E+06

TABLE A-1b-38

CHEMICAL-SPECIFIC INPUTS FOR 3-METHYLCHOLANTHRENE (56-49-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	2.60E+01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	2.60E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-39

CHEMICAL-SPECIFIC INPUTS FOR METHYL METHACRYLATE (80-62-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	100.13
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.10E-02
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.60E+04
H (atm·m^3/mol)	U.S. EPA (1995g)	3.20E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.70E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.60E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.40E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.30E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.30E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.72E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.50E-03
t	*t* value was obtained from U.S. EPA (1992b).	3.60E-01
*t**	t* value was obtained from U.S. EPA (1992b).	8.60E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.40E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.2E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-39

CHEMICAL-SPECIFIC INPUTS FOR METHYL METHACRYLATE (80-62-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	8.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	2.80E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-40

CHEMICAL-SPECIFIC INPUTS FOR 2-METHYLNAPTHALENE (91-57-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	142.20
T_m (K)	CRC Handbook (1995)	307.55
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.05E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.84E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.42E-01
t	*t* value was obtained from U.S. EPA (1992b).	6.44E-01
*t**	t* value was obtained from U.S. EPA (1992b).	4.87E+00
B	*B* value was obtained from U.S. EPA (1992b).	7.24E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-40

CHEMICAL-SPECIFIC INPUTS FOR 2-METHYLNAPTHALENE (91-57-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-41

CHEMICAL-SPECIFIC INPUTS FOR MOLYBDENUM (7439-98-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	95.94
T_m (K)	--	N/A
Vp (atm)	--	N/A
S (mg/L)	--	N/A
H (atm·m^3/mol)	--	N/A
D_a (cm^2/s)	--	N/A
D_w (cm^2/s)	--	N/A
K_{ow} (unitless)	--	N/A
K_{oc} (mL/g)	--	N/A
Kd_s (cm^3/g)	U.S. EPA (1995g)	2.00E+01
Kd_{sw} (L/Kg)	--	2.00E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
t	*t* value was obtained from U.S. EPA (1992b).	ND
*t**	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-41

CHEMICAL-SPECIFIC INPUTS FOR MOLYBDENUM (7439-98-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	5.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1996c)	2.40E+00

Note: NA= Not applicable, ND= No data available

TABLE A-1b-42

CHEMICAL-SPECIFIC INPUTS FOR 1,4-NAPHTHAQUINONE (130-15-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	158.15
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	399.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.60E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.98E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.39E-03
t	*t* value was obtained from U.S. EPA (1992b).	8.05E-01
*t**	t* value was obtained from U.S. EPA (1992b).	1.93E+00
B	*B* value was obtained from U.S. EPA (1992b).	5.13E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-42

CHEMICAL-SPECIFIC INPUTS FOR 1,4-NAPHTHAQUINONE (130-15-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-43

CHEMICAL-SPECIFIC INPUTS FOR 2-NAPHTHYLAMINE (91-59-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	143.18
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	323.15
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	U.S. EPA (1995g)	6.03E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.51E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.39E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
t	*t* value was obtained from U.S. EPA (1992b).	6.50E-01
*t**	t* value was obtained from U.S. EPA (1992b).	1.60E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.90E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.70E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-43

CHEMICAL-SPECIFIC INPUTS FOR 2-NAPHTHYLAMINE (91-59-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-44

CHEMICAL-SPECIFIC INPUTS FOR 5-NITRO-O-TOLUIDINE (2-METHYL-5-NITROANILINE) (99-55-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	152.15
T_m (K)	CRC Handbook (1995)	378.65
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.78E-03
t	*t* value was obtained from U.S. EPA (1992b).	7.41E-01
*t**	t* value was obtained from U.S. EPA (1992b).	1.78E+00
B	*B* value was obtained from U.S. EPA (1992b).	7.41E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-44

CHEMICAL-SPECIFIC INPUTS FOR 5-NITRO-O-TOLUIDINE (2-METHYL-5-NITROANILINE) (99-55-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA= Not applicable, ND= No data available

TABLE A-1b-45

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPROPANE (79-46-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	89.09
T_m (K)	U.S. EPA (1995g)	NA
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	2.40E-02
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.70E+05
H (atm·m^3/mol)	U.S. EPA (1995g)	1.23E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.23E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.01E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g)	7.40E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.20E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.20E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.40E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.30E-03
t	*t* value was obtained from U.S. EPA (1992b).	3.10E-01
*t**	t* value was obtained from U.S. EPA (1992b).	7.30E-01
B	*B* value was obtained from U.S. EPA (1992b).	7.40E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	7.20E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-45

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPROPANE (79-46-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	Calculated from *RfC* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	5.70E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (1997b)	2.00E-02
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	9.40E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA= Not applicable, ND= No data available

TABLE A-1b-46

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROQUINOLINE-1-OXIDE (56-57-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	190.16
T_m (K)	CRC Handbook (1995)	427.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	8.00E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.00E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
t	*t* value was obtained from U.S. EPA (1992b).	4.40E-01
*t**	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	NA
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-46

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROQUINOLINE-1-OXIDE (56-57-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-47

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIETHYLAMINE (55-18-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	102.14
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	2.60E-03
S (mg/L)	U.S. EPA (1995g)	2.00E+05
H (atm·m^3/mol)	U.S. EPA (1995g)	3.63E-06
D_a (cm^2/s)	U.S. EPA (1995g)	8.00E-02
D_w (cm^2/s)	U.S. EPA (1995g)	8.00E-06
K_{ow} (unitless)	U.S. EPA (1995g)	3.00E+00
K_{oc} (mL/g)	U.S. EPA (1995g)	3.00E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.00E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.10E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	9.90E-04
t	*t* value was obtained from U.S. EPA (1992b).	3.70E-01
*t**	t* value was obtained from U.S. EPA (1992b).	8.80E-01
B	*B* value was obtained from U.S. EPA (1992b).	3.00E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1995g)	6.30E-01
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-47

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIETHYLAMINE (55-18-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	1.52E+02
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	1.52E+02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-48

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIMETHYLAMINE (62-75-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	74.08
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.10E-03
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.00E+06
H (atm·m^3/mol)	U.S. EPA (1995g)	5.30-E07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.70E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.80E-01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.80E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.10E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.70E-04
t	*t* value was obtained from U.S. EPA (1992b).	2.50E-01
*t**	t* value was obtained from U.S. EPA (1992b).	5.90E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.70E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	7.40E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-48

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIMETHYLAMINE (62-75-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	5.10E+01
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EAP (1997c)	4.90E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-49

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOMETHYLETHYLAMINE (10595-95-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	88.13
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.00E-03
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.00E+05
H (atm·m^3/mol)	U.S. EPA (1995g)	8.90E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	7.60E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.60E-01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.60E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.70E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.50E-04
t	*t* value was obtained from U.S. EPA (1992b).	3.00E-01
*t**	t* value was obtained from U.S. EPA (1992b).	7.20E-01
B	*B* value was obtained from U.S. EPA (1992b).	7.60E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.10E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-49

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOMETHYLETHYLAMINE (10595-95-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	2.20E+01
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	2.20E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA= Not applicable, ND= No data available

TABLE A-1b-50

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOMORPHOLINE (59-89-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	116.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	302.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.00E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
t	*t* value was obtained from U.S. EPA (1992b).	4.50E-01
*t**	t* value was obtained from U.S. EPA (1992b).	1.10E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.60E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-50

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOMORPHOLINE (59-89-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA= Not applicable, ND= No data available

TABLE A-1b-51

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOPIPERIDINE (100-75-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	114.5
T_m (K)	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.90E-04
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.50E+05
H (atm·m^3/mol)	U.S. EPA (1995g)	1.40E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	4.30E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.20E+00
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.20E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.15E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-03
t	*t* value was obtained from U.S. EPA (1992b).	4.40E-01
*t**	t* value was obtained from U.S. EPA (1992b).	1.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.30E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	8.20E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-51

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOPIPERIDINE (100-75-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	3.80E+01
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	3.80E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-52

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOPYRROLIDINE (930-55-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	100.11
T_m (K)	--	
Vp (atm)	*Vp* value cited in Montgomery and Weldom (1991).	2.30E-04
S (mg/L)	*S* value cited in U.S. EPA (1995g).	7.80E+05
H (atm·m^3/mol)	U.S. EPA (1995g)	2.90E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.36E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.04E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	6.50E-01
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	6.50E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.50E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.90E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.40E-04
t	*t* value was obtained from U.S. EPA (1992b).	3.60E-01
*t**	t* value was obtained from U.S. EPA (1992b).	8.60E-01
B	*B* value was obtained from U.S. EPA (1992b).	6.50E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.90E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-52

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOPYRROLIDINE (930-55-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S.EPA (1997b)	2.10E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	2.10E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-53

CHEMICAL-SPECIFIC INPUTS FOR OCTAMETHYLPYROPHOSPHORAMIDE (152-16-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	286.26
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.30E-06
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.00E+06
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	3.80E-10
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.62E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	3.00E-01
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	3.10E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.10E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.30E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.50E-05
t	*t* value was obtained from U.S. EPA (1992b).	4.90E+00
*t**	t* value was obtained from U.S. EPA (1992b).	1.20E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.00E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.00E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-53

CHEMICAL-SPECIFIC INPUTS FOR OCTAMETHYLPYROPHOSPHORAMIDE (152-16-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1997b)	2.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.00E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-54

CHEMICAL-SPECIFIC INPUTS FOR PARATHION (ETHYL) (56-38-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	291.27
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.30E-08
S (mg/L)	*S* value cited in U.S. EPA (1995g).	6.50E+00
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	5.70E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.70E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.79E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	6.80E+03
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	5.80E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.80E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.35E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.70E-02
t	*t* value was obtained from U.S. EPA (1992b).	5.20E+00
*t**	t* value was obtained from U.S. EPA (1992b).	3.90E+01
B	*B* value was obtained from U.S. EPA (1992b).	6.80E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.70E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-54

CHEMICAL-SPECIFIC INPUTS FOR PARATHION (ETHYL) (56-38-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	6.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	2.10E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.3E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1b-55

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROETHANE (76-01-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	202.31
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	244.15
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.815E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.60E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.30E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.63E-02
t	*t* value was obtained from U.S. EPA (1992b).	1.50E+00
*t**	t* value was obtained from U.S. EPA (1992b).	4.05E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.12E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-55

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROETHANE (76-01-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)		ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-56

CHEMICAL-SPECIFIC INPUTS FOR PHENACETIN (62-44-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	179.21
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	407.15 to 408.15
Vp (atm)	--	ND
S (g/1310ml of H_2O)	*S* value cited in U.S. EPA (1995b).	1.0
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.41E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.70E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.82E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.03E-03
t	*t* value was obtained from U.S. EPA (1992b).	1.08E+00
*t**	t* value was obtained from U.S. EPA (1992b).	2.60E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.80E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-56

CHEMICAL-SPECIFIC INPUTS FOR PHENACETIN (62-44-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA= Not applicable, ND= No data available

TABLE A-1b-57

CHEMICAL-SPECIFIC INPUTS FOR PHENYL MERCURIC ACETATE (62-38-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	336.75
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	4.00E-09
S (mg/L)	*S* value cited in U.S. EPA (1995g).	4.40E+03
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	2.04E-11
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.58E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.62E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	1.70E+02
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	1.60E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.60E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.20E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	6.40E-04
t	*t* value was obtained from U.S. EPA (1992b).	9.90E+00
*t**	t* value was obtained from U.S. EPA (1992b).	2.40E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.70E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1995g)	1.50E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-57

CHEMICAL-SPECIFIC INPUTS FOR PHENYL MERCURIC ACETATE (62-38-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S.EPA (1997b)	8.00E-05
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	2.80E-04
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-58

CHEMICAL-SPECIFIC INPUTS FOR 1,3-PHENYLENEDIAMINE (108-45-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	108.6
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	3.00E-05
S (mg/L)	*S* value cited in U.S. EPA (1995g).	3.50E+05
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	9.20E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.63E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.88E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	1.10E+00
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	1.10E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.10E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.25E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.50E-04
t	*t* value was obtained from U.S. EPA (1992b).	4.00E-01
*t**	t* value was obtained from U.S. EPA (1992b).	9.60E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.10E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	U.S. EPA (1995g)	2.90E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-58

CHEMICAL-SPECIFIC INPUTS FOR 1,3-PHENYLENEDIAMINE (108-45-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	6.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	2.10E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-59

CHEMICAL-SPECIFIC INPUTS FOR A-PICOLINE (109-06-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	93.12
T_m (°K)	--	203.15
Vp (mm@°C)	*Vp* value cited in U.S. EPA (1995g).	8.00E+00
S (mg/L)	*S* value cited in U.S. EPA (1995g).	
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	4.10E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.50E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.60E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	2.00E+06
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	1.50E+06
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.50E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.12E+05
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.16E-03
t	*t* value was obtained from U.S. EPA (1992b).	3.24E-01
*t**	t* value was obtained from U.S. EPA (1992b).	7.76E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.29E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-59

CHEMICAL-SPECIFIC INPUTS FOR A-PICOLINE (109-06-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA= Not applicable, ND= No data available

TABLE A-1b-60

CHEMICAL-SPECIFIC INPUTS FOR POLYCHLORINATED BIPHENYLS (AROCLORS) (1336-36-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	328
T_m (^{o}K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.00E-07
S (mg/L)	*S* value cited in U.S. EPA (1995g).	8.00E-02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	2.60E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.00E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	2.00E+06
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1998c).	9.83E+04
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.83E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.37E+03
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.30E+00
t	*t* value was obtained from U.S. EPA (1992b).	5.30E+00
*t**	t* value was obtained from U.S. EPA (1992b).	2.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.20E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)		6.70E+05

TABLE A-1b-60

CHEMICAL-SPECIFIC INPUTS FOR POLYCHLORINATED BIPHENYLS (AROCLORS) (1336-36-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	2.00E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	2.00E+00
MCL	National Primary Drinking Water Regulations.	5E-04
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.4E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1b-61

CHEMICAL-SPECIFIC INPUTS FOR TETRAETHYL DITHIOPYROPHOSPHATE (SULFOTEP) (3689-24-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	322.31
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	3.30E-07
S (mg/L)	*S* value cited in U.S. EPA (1995g).	2.50E+01
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	4.20E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	6.80E+03
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	5.80E+03
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.80E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.35E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
t	*t* value was obtained from U.S. EPA (1992b).	8.10E+00
*t**	t* value was obtained from U.S. EPA (1992b).	6.00E+01
B	*B* value was obtained from U.S. EPA (1992b).	6.80E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1995g)	2.80E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-61

CHEMICAL-SPECIFIC INPUTS FOR TETRAETHYL DITHIOPYROPHOSPHATE (SULFOTEP) (3689-24-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	5.00E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.75E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-62

CHEMICAL-SPECIFIC INPUTS FOR THIONAZIN (297-97-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	248.26
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	271.45
Vp (mmHg)	U.S. EPA (1995g)	3.00E-03
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.60E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
t	*t* value was obtained from U.S. EPA (1992b).	2.86E+00
*t**	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-62

CHEMICAL-SPECIFIC INPUTS FOR THIONAZIN (297-97-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-63

CHEMICAL-SPECIFIC INPUTS FOR TIN (7440-31-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	118.69
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	505.05
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
t	*t* value was obtained from U.S. EPA (1992b).	ND
*t**	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-63

CHEMICAL-SPECIFIC INPUTS FOR TIN (7440-31-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	6.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	2.10E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-64

CHEMICAL-SPECIFIC INPUTS FOR 2,4-TOLUENEDIAMINE (95-80-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	122.17
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.10E-07
S (mg/L)	*S* value cited in U.S. EPA (1995g).	7.50E+03
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	7.92E-10
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.05E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	2.50E+00
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	2.50E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.50E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.88E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	6.60E-04
t	*t* value was obtained from U.S. EPA (1992b).	4.90E-01
*t**	t* value was obtained from U.S. EPA (1992b).	1.20E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.50E-04
Biotransfer Factors for Animals		
BCF_{fish} (unitless FW tissue)	U.S. EPA (1995g)	4.60E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-64

CHEMICAL-SPECIFIC INPUTS FOR 2,4-TOLUENEDIAMINE (95-80-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	3.20E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	3.20E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note:NA = Not applicable, ND = No data available

TABLE A-1b-65

CHEMICAL-SPECIFIC INPUTS FOR P-TOLUIDINE (106-49-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	107.15
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	317.65
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	4.30E-04
S (mg/L)	*S* value cited in U.S. EPA (1995g).	7.60E+03
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	6.10E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.97E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.43E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	2.50E+01
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	2.40E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.40E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.80E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.20E-03
t	*t* value was obtained from U.S. EPA (1992b).	3.90E-01
*t**	t* value was obtained from U.S. EPA (1992b).	9.50E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.50E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1995g)	3.50E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-65

CHEMICAL-SPECIFIC INPUTS FOR P-TOLUIDINE (106-49-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997b)	1.90E-01
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	1.90E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-66

CHEMICAL-SPECIFIC INPUTS FOR TOXAPHENE (CHLORINATED CAMPHENES) (8001-35-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	414
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	350.65
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	4.30E-04
S (mg/L)	*S* value cited in U.S. EPA (1995g).	6.79E-01
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	3.40E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.16E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.34E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	3.20E+05
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	2.60E+05
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.60E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.95E+04
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.60E-02
t	*t* value was obtained from U.S. EPA (1992b).	2.90E+01
*t**	t* value was obtained from U.S. EPA (1992b).	1.40E+02
B	*B* value was obtained from U.S. EPA (1992b).	3.20E+01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	(U.S. EPA 1995g)	2.10E+06

TABLE A-1b-66

CHEMICAL-SPECIFIC INPUTS FOR TOXAPHENE (CHLORINATED CAMPHENES) (8001-35-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	1.10E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	1.10E+00
MCL	National Primary Drinking Water Regulations.	3E-03
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	2E-04

Note: NA = Not applicable, ND = No data available

TABLE A-1b-67

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE (76-13-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	187.38
T_m (^{o}K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	4.80E-01
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.70E+02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	4.815E-01
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.20E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	1.40E+03
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	1.30E+03
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.30E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.81E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.40E-02
t	*t* value was obtained from U.S. EPA (1992b).	1.20E+00
*t**	t* value was obtained from U.S. EPA (1992b).	4.10E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.40E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	8.20E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-67

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE (76-13-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	3.00E+01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (1997c)	8.57E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-68

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROPHENOXY PROPIONIC ACID (SILVEX) (93-72-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	269.51
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	6.80E-09
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.40E+02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	1.30E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	2.60E+03
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	2.30E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.30E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.71E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
t	*t* value was obtained from U.S. EPA (1992b).	3.90E+00
*t**	t* value was obtained from U.S. EPA (1992b).	1.90E+01
B	*B* value was obtained from U.S. EPA (1992b).	2.60E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.30E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-68

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROPHENOXY PROPIONIC ACID (SILVEX) (93-72-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	8.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	2.80E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	5E-02
Aquatic TRV (µg/l)	--.	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-69

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOXYACETIC ACID (93-76-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	255.49
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	9.10E-10
S (mg/L)	*S* value cited in U.S. EPA (1995g).	2.80E+02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	8.68E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	2.00E+03
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	1.80E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.80E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.35E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.20E-02
t	*t* value was obtained from U.S. EPA (1992b).	3.20E+00
*t**	t* value was obtained from U.S. EPA (1992b).	1.30E+01
B	*B* value was obtained from U.S. EPA (1992b).	2.00E-01
Biotransfer Factors for Animals		
BCF_{fish} (unitless FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	7.80E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-69

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOXYACETIC ACID (93-76-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997a)	1.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.50E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note:NA = Not applicable, ND = No data available

TABLE A-1b-70

CHEMICAL-SPECIFIC INPUTS FOR O,O,O-TRIETHYLPHOSPHOROTHIATE (126-68-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	198.22
T_m (°K)	--	ND
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	3.17E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.23E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (mL/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
t	*t* value was obtained from U.S. EPA (1992b).	1.42E+00
*t**	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1b-70

CHEMICAL-SPECIFIC INPUTS FOR O,O,O-TRIETHYLPHOSPHOROTHIATE (126-68-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (water) (mg/kg/day)	--	ND
RfD (food) (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-71

CHEMICAL-SPECIFIC INPUTS FOR TRIS(2,3-DIBROMOPROPYL) PHOSPHATE B19 (126-72-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	697.93
T_m (K)	--	ND
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	2.00E-07
S (mg/L)	*S* value cited in U.S. EPA (1995g).	4.70E+00
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	3.00E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.50E-03
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.66E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	3.20E+03
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	2.80E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.80E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.10E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.30E-05
t	*t* value was obtained from U.S. EPA (1992b).	1.60E+03
*t**	t* value was obtained from U.S. EPA (1992b).	8.60E+03
B	*B* value was obtained from U.S. EPA (1992b).	3.20E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.60E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-71

CHEMICAL-SPECIFIC INPUTS FOR TRIS(2,3-DIBROMOPROPYL) PHOSPHATE B19 (126-72-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	9.80E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	9.80E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1b-72

CHEMICAL-SPECIFIC INPUTS FOR VANADIUM (7440-62-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	--	50.94
T_m (K)	--	
Vp (atm)	--	N/A
S (mg/L)	--	N/A
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
K_{ow} (unitless)	--	N/A
K_{oc} (mL/g)	--	N/A
Kd_s (cm^3/g)	U.S. EPA (1995g)	5.00E+01
Kd_{sw} (L/Kg)	--	5.00E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
t	--	ND
*t**	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-72

CHEMICAL-SPECIFIC INPUTS FOR VANADIUM (7440-62-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	7.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	2.45E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1996c)	1.9E+01

Note:NA = Not applicable, ND = No data available

TABLE A-1b-73

CHEMICAL-SPECIFIC INPUTS FOR XYLENES (TOTAL) (1330-20-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.17
T_m (^{o}K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.10E-02
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.90E+02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	6.00E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.14E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.34E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	1.50E+03
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	1.30E+03
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.30E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.75E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	7.60E-02
t	*t* value was obtained from U.S. EPA (1992b).	3.90E-01
*t**	t* value was obtained from U.S. EPA (1992b).	1.30E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.50E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	7.50E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1b-73

CHEMICAL-SPECIFIC INPUTS FOR XYLENES (TOTAL) (1330-20-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997b)	2.00E+00
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.00E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	1.0E+01
Aquatic TRV (µg/l)	U.S. EPA (1996c)	1.80E+00

Note: Not applicable, ND = No data available